

Bound-states in dimerized and frustrated Heisenberg Chains

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Using the Bond Operator Technique (BOT), we have studied the low energy excitation spectrum of a frustrated dimerized antiferromagnetic Heisenberg chain. In particular, we have compared our analytical results with previous Exact Diagonalizations (ED) data. Qualitatively, the BOT results are in good agreement with the ED data. And even a very good quantitative agreement is obtained in some parameter region. It is clearly shown that there is only one elementary excitation branch (lowest triplet branch) and that the two other well defined excitations which appear below the continuum, one singlet and one triplet, are bound states of two elementary triplets.

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I. INTRODUCTION

The magnetic properties of low dimensional quantum spin systems have attracted a considerable attention of theorists over the last decades. The interest for these systems was boosted by the recent discovery of non organic spin-Peierls materials like CuGeO_3 [1] and NaV_2O_5 [2,3] and spin ladder compounds like SrCu_2O_3 , $\text{Sr}_2\text{Cu}_3\text{O}_5$ [4,5]. It turns out that some of the properties of these materials can be described by the frustrated dimerized Heisenberg model. In the one dimensional case, the Hamiltonian of this model reads,

$$H = J \sum_i ([1 + \delta(-1)^i] \mathbf{S}_i \cdot \mathbf{S}_{i+1} + \alpha \mathbf{S}_i \cdot \mathbf{S}_{i+2}) \quad (1)$$

where i denotes the sites of a chain with length L and \mathbf{S}_i are $S = 1/2$ spin operators. $J > 0$ is the nearest-neighbor exchange coupling, α the frustration parameter from next-nearest neighbor coupling and δ is the dimerization parameter.

Depending on the coupling parameters, this model exhibits various phases including spin-liquid phase (gapless phase), dimerized phase, Neel ordered phase and incommensurate phase. The ground-state properties of this model were extensively studied using various numerical and analytical tools, like Exact Diagonalizations method, Quantum Monte Carlo, DMRG (density matrix renormalization group), Bethe ansatz, bond operator technique, etc.. Another interesting feature of the frustrated dimerized Heisenberg model is the possible existence of well defined excited states below the continuum (bound-states?) [6–9]. Recently, Bouzerar et al. have provided a detailed numerical analysis (Exact diagonalizations method) of the excitation spectrum in this model [8]. It was shown that: (i) The Singlet-Triplet excitation gap ratio is a universal function which depends on the frustration parameter only and (ii) A well defined second triplet branch appears below the continuum in the vicinity of momentum $q = 0$ (resp. π) only if the strength of the frustration is large enough. A useful approach to describe

the dimerized phase is the Bond-Operator representation of spins introduced by Chubukov [10] and Sachdev and Bhatt [11]. Recently a number of works have been carried out with the help of bond-operator method. Employing the bond-operator methodology Brenig [12] studied the effect of interchain coupling in spin-Peierls systems like CuGeO_3 . This method was also successfully used by Sushkov and Kotov to spin ladder model in the strong interchain coupling limit $J_\perp \gg J_\parallel$, to show the existence of a singlet and triplet bound states below the continuum [14]. In this paper we will study the excited states of the frustrated dimerized Heisenberg model using the Bond-Operator Technique (BOT) and compare the results of our calculation with the Exact Diagonalizations data (ED) [8]. We will show that the agreement between ED and BOT is very good at least qualitatively, and even quantitatively in the vicinity of momentum $q = \pi/2$. We will also show that the lowest triplet branch is the only elementary excitation and that the singlet and the triplet which appear below the continuum are bound-states of two triplets.

II. BOND OPERATOR TECHNIQUE

In this method the Hilbert space of the spin degrees of freedom is represented in terms of singlet and three triplet states which is created out of vacuum by one singlet (s^\dagger) and three triplets (t^\dagger) creation operators

$$\begin{aligned} |s_i\rangle &= s_i^\dagger |0\rangle = \frac{1}{\sqrt{2}} (|\uparrow_{2i}\downarrow_{2i+1}\rangle - |\downarrow_{2i}\uparrow_{2i+1}\rangle), \\ |t_{xi}\rangle &= t_{xi}^\dagger |0\rangle = -\frac{1}{\sqrt{2}} (|\uparrow_{2i}\uparrow_{2i+1}\rangle - |\downarrow_{2i}\downarrow_{2i+1}\rangle), \\ |t_{yi}\rangle &= t_{yi}^\dagger |0\rangle = \frac{i}{\sqrt{2}} (|\uparrow_{2i}\uparrow_{2i+1}\rangle + |\downarrow_{2i}\downarrow_{2i+1}\rangle), \\ |t_{zi}\rangle &= t_{zi}^\dagger |0\rangle = \frac{1}{\sqrt{2}} (|\uparrow_{2i}\downarrow_{2i+1}\rangle + |\downarrow_{2i}\uparrow_{2i+1}\rangle). \end{aligned} \quad (2)$$

A representation of spins in terms of the singlet and triplet operators is given by

$$\begin{aligned}
S_{\alpha 2i} &= \frac{1}{2}(s_i^\dagger t_{\alpha i} + t_{\alpha i}^\dagger s_i - i\epsilon_{\alpha\beta\gamma} t_{\beta i}^\dagger t_{\gamma i}), \\
S_{\alpha 2i+1} &= \frac{1}{2}(-s_i^\dagger t_{\alpha i} - t_{\alpha i}^\dagger s_i - i\epsilon_{\alpha\beta\gamma} t_{\beta i}^\dagger t_{\gamma i}),
\end{aligned} \quad (3)$$

where α, β and $\gamma = x, y, z$ and $\epsilon_{\alpha\beta\gamma}$ is the Levi-Civita symbol representing the totally antisymmetric tensor. Henceforth it is assumed that all repeated indices over α, β and γ are summed over. The four operators (s, t_x, t_y and t_z) satisfy the usual bosonic commutation relations. In order to ensure that the physical states are either singlet or triplets one has to impose the constraint

$$s_i^\dagger s_i + t_{\alpha i}^\dagger t_{\alpha i} = 1. \quad (4)$$

It is a difficult task to fulfill this constraint exactly (in each bond) and in most of the works this constraint is satisfied only in average. To overcome this difficulty, an infinite on site repulsion has been introduced by Kotov et al. [13]. In Bond-operator representation the Hamiltonian reads,

$$H = H_0 + H_1 + H_2 \quad (5)$$

$$\begin{aligned}
H_0 &= -\frac{3}{4}J(1+\delta)\frac{L}{2} + J(1+\delta) \sum_{i=1, \alpha}^{\frac{L}{2}} t_{\alpha i}^\dagger t_{\alpha i} \\
&\quad - K_0 \sum_{i=1}^{\frac{L}{2}} (t_{\alpha i}^\dagger t_{\alpha i+1} s_i^\dagger s_{i+1} + t_{\alpha i}^\dagger t_{\alpha i+1}^\dagger s_i s_{i+1} + h.c) \\
H_1 &= K_1 \sum_{i=1, \alpha \neq \beta}^{\frac{L}{2}} (t_{\alpha i}^\dagger t_{\beta i+1}^\dagger t_{\beta i} t_{\alpha i+1} - t_{\alpha i}^\dagger t_{\alpha i+1}^\dagger t_{\beta i} t_{\beta i+1}) \\
H_2 &= K_2 \sum_{i=1, \alpha, \beta, \gamma}^{\frac{L}{2}} (i\epsilon_{\alpha\beta\gamma} [t_{\alpha i}^\dagger t_{\beta i+1}^\dagger t_{\gamma i+1} s_i \\
&\quad - t_{\alpha i+1}^\dagger t_{\beta i}^\dagger t_{\gamma i} s_{i+1}] + h.c)
\end{aligned}$$

with $K_0 = \frac{J}{4}(1-\delta-2\alpha), K_1 = \frac{J}{4}(1-\delta+2\alpha)$ and $K_2 = \frac{J}{4}(1-\delta)$.

This method gives the exact ground-state in the limit when the ground state wave function consists of a product of local independent dimers which is especially realized on the 'disordered line' $2\alpha + \delta = 1$. On this line the Ground-state energy per site is $E_G/L = -\frac{3}{8}(1+\delta)$. It should be noted that in the BOT the elementary excitation is a local triplet (nearest neighbor sites).

In order to perform the calculation of the triplet dispersion: (i) Initially we neglect completely the local constraint which is equivalent to set $s_i = 1$. (ii) We restrict ourself to the quadratic terms only. As it was previously shown that the effect of the higher order terms H_1 and H_2 are small [15,11].

After using the well known Bogoliubov transformation $t_{\alpha k} = u_k a_{\alpha k} + v_k a_{-\alpha k}^\dagger$, the hamiltonian reduces to,

$$H = -\frac{9}{8}J(1+\delta)L + \sum_{\alpha, k=-\frac{\pi}{2}}^{\frac{\pi}{2}} \omega_k (a_{\alpha k}^\dagger a_{\alpha k} + \frac{1}{2}) \quad (6)$$

where

$$\begin{aligned}
\omega_k &= \sqrt{A_k^2 - B_k^2} \\
u_k &= \sqrt{\frac{1}{2} + \frac{A_k}{2\omega_k}} \\
v_k &= \sqrt{-\frac{1}{2} + \frac{A_k}{2\omega_k}}
\end{aligned} \quad (7)$$

with $A_k = J(1+\delta) - \frac{J}{2}(1-\delta-2\alpha)\cos(2k)$ and $B_k = -\frac{J}{2}(1-\delta-2\alpha)\cos(2k)$.

Let us now take into account the effect of the local constraint eq. (4). Following the ref. [13] we include in the previous Hamiltonian an infinite on site repulsion H_U ,

$$H_U = U \sum_{i, \alpha\beta} t_{\alpha i}^\dagger t_{\beta i}^\dagger t_{\beta i} t_{\alpha i}, \quad U \rightarrow \infty \quad (8)$$

Concerning the calculation of the self-energy correction to the dispersion we follow the diagrammatic approach developed in ref. [13]. Let us just summarize the main steps of the calculation. At first the vertex scattering amplitude $\Gamma(k, \omega)$ is evaluated by solving the Bethe-Salpeter equation shown in fig.1 a.

$$\begin{aligned}
\Gamma(k, \omega) &= [i \int dq d\omega' G(q, \omega') G(k-q, \omega-\omega')]^{-1} \\
&= -[\frac{1}{N} \sum_q \frac{u_q^2 u_{k-q}^2}{\omega - \omega_q - \omega_{k-q}} + \{u \rightarrow v, \omega \rightarrow -\omega\}]^{-1}
\end{aligned} \quad (9)$$

where $G(k, \omega)$ is the normal Greens function of H_0 . We neglect the higher order terms of v_q since $\sum_q v_q^2$ is proportional to the number of triplets in the system and it is very small in the dimerized phase.

Then taking the scattering vertex as $\Gamma(k, \omega)$, the corresponding self energy is obtained from the diagram shown in fig 1 b,

$$\Sigma(k, \omega) = \frac{8}{N} \sum_{q=-\frac{\pi}{2}}^{\frac{\pi}{2}} v_q^2 \Gamma(k+q, \omega-\omega_q). \quad (10)$$

Now we calculate the renormalized spectrum

$$\Omega_k = Z_k \sqrt{((A_k + \Sigma(k, 0))^2 - B_k^2)} \quad (11)$$

from the poles of the modified Greens function. Here the quasiparticle weight

$$Z_k = (1 - \frac{\partial \Sigma}{\partial \omega})^{-1} \quad (12)$$

III. SINGLET-TRIPLET GAP AND DISPERSION

In this section we will compare the BOT results (with and without the constraint) of the Singlet-Triplet gap and Dispersion to the ED data of ref. [8]. We observe in fig. 1, that the gap Δ_{BOT} is always larger than the exact result and even gets worse when the constraint is included. For a given δ , the difference between the gaps with and without constraint reduces when it approaches the disordered line. On the disordered line, it can be seen easily from equation (11), that the dispersion is unchanged when the constraint is included, since $\Sigma(k, \omega) \propto (2\alpha + \delta - 1)$. However, the agreement between BOT and ED gets better in the limit of large δ . For instance at $\alpha = 0$, we get $\frac{\Delta_{ED}}{\Delta_{BOT}} = 0.67$ for $\delta = 0.2$, but this ratio is 0.87 when $\delta = 0.4$. This ratio increases with α . Furthermore, the curve including the constraint is parallel to the ED data curve, this means that the effect of frustration is taken into account more properly when the constraint is included. However, in the limit of vanishing δ the effect of frustration is not taken properly in the BOT approach [12]. For instance at the Majumdar-Ghosh [16] point ($\alpha = 0.5, \delta = 0$), $\frac{\Delta_{ED}}{\Delta_{BOT}} \approx 0.25$.

Let us now discuss the dispersion of the triplet excitation ($\omega(q)$). In order to analyze the effect of the frustration on $\omega(q)$ we have fixed the dimerization parameter $\delta = 0.2$. In fig. 3 a (resp. 3 b) we have plotted the dispersion for $\alpha = 0$ (resp. $\alpha = 0.3$). In fig. 3 a and fig. 3 b we observe that the agreement between the ED data and BOT with constraint are excellent in the vicinity of $q = \pi/2$. This agreement will get better with increasing δ . Note that on the disordered line the BOT data coincides exactly with the ED data. Indeed, on this line and at $q = \pi/2$, the lowest triplet excitation is $|T(\pi/2)\rangle = \sum_l e^{i\frac{\pi}{2}l} S_l^\dagger |GS\rangle$, where the ground-state wave function $|GS\rangle$ consists of product of independent dimers [17]. Note that even far from the disordered line, this state remains a good approximation of the exact lowest triplet state in the vicinity of $\pi/2$. It is important to emphasize, that away from $q = \pi/2$, the disagreement between BOT and ED data is mainly due to the fact that the *triplet excitation are not local objects*, but in the BOT scheme by construction the triplet excitation are local. We observe in fig. 3 a (resp. 3 b) that when approaching the disordered line the width of the dispersion strongly decreases, and the agreement with the ED data gets worse. On the disordered line, the BOT triplet excitation is dispersionless and $\omega(q) = J(1 + \delta)$. However, as discussed previously, when δ is increased the agreement between BOT and ED gets better and better and coincide for the special case $\delta = 1$ and $\alpha = 0$.

IV. TWO MAGNONS BOUND-STATE.

The quartic term H_1 in the Hamiltonian eq. 5, consist of triplet-triplet interaction. This term can lead to

an attractive interaction between triplets to form bound-states. This bound-states can be singlet, triplet or quintuplet. We will focus only on the possibility of a singlet or triplet bound-states which were observed below the continuum in the ED calculations [8]. In the previous section we have seen that the effect of the constraint does not significantly modify the triplet dispersion, thus to simplify the calculations we will neglect the constraint.

A. Singlet bound-state.

To perform the calculation of the singlet bound-state, let us consider the most general singlet wave function

$$|\Psi^S(Q)\rangle = \sum_{k,\alpha} \Phi^S(k) a_{\alpha Q/2-k}^\dagger a_{\alpha Q/2+k}^\dagger |0\rangle \quad (13)$$

of total momentum Q , constructed from two triplet elementary excitations, where $\Phi^S(k)$ is determined from the Schrödinger equation,

$$H|\Psi^S(Q)\rangle = E^S(Q)|\Psi^S(Q)\rangle \quad (14)$$

with singlet bound state energy $E^S(Q)$. This leads immediately to the integral equation of the form,

$$(E^S(Q) - \omega_{Q/2-q} - \omega_{Q/2+q})\Phi^S(q) = -4K_1 g(q) \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \frac{dp}{\pi} g(p) \Phi^S(p) \quad (15)$$

where $g(p) = \cos(2p)u_{Q/2-p}u_{Q/2+p}$.

In the vicinity of the disordered line ($|2\alpha + \delta - 1| \ll 1$) this integral can be solved analytically. In this region of parameter $u_k \approx 1$ and $\omega_k/J \approx (1 + \delta) - \frac{1}{2}(1 - \delta - 2\alpha)\cos(2k)$. The corresponding singlet energy for the momentum Q is,

$$E^S(Q)/J = 2(1 + \delta) - \frac{1}{2}\sqrt{(1 - \delta + 2\alpha)^2 + 4(1 - \delta - 2\alpha)^2\cos^2(Q)}. \quad (16)$$

For any momentum Q the energy of the singlet state is always smaller than the energy of the lower edge of the continuum defined as $E^C(Q) = \min_q(\omega_{Q/2-q} + \omega_{Q/2+q}) = 2(1 + \delta) - |(1 - \delta - 2\alpha)\cos(Q)|$. Thus, a well defined singlet bound-state exists for any momentum Q . Far from the disordered line the equation (15) should be solved numerically.

B. Triplet bound-state.

Let us now perform analogous calculations in the triplet sector. The most general triplet wave function can be written,

$$|\Psi_\alpha^T(Q)\rangle = \sum_{k,\beta\gamma} \Phi_\alpha^T(k) \epsilon_{\alpha\beta\gamma} a_{\beta Q/2-k}^\dagger a_{\gamma Q/2+k}^\dagger |0\rangle \quad (17)$$

The corresponding Schrödinger equation is,

$$(E^T(Q) - \omega_{Q/2-q} - \omega_{Q/2+q})\Phi_\alpha^T(q) = -2K_1 h(q) \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \frac{dp}{\pi} h(p) \Phi_\alpha^T(p) \quad (18)$$

where $h(p) = \sin(2p)u_{Q/2-p}u_{Q/2+p}$.

As we did it previously, we solve this equation analytically in the vicinity of the disordered line. We get,

$$E^T(Q)/J = 2(1 + \delta) - K_1[1 + (\frac{2K_0}{K_1})^2 \cos^2(Q)] \quad (19)$$

We find that the Triplet is below the continuum (i.e. $E^T(Q) < E^C(Q)$) when $Q > Q_c$, where

$$Q_c = \cos^{-1}[\frac{1 - \delta + 2\alpha}{2(1 - \delta - 2\alpha)}] \quad (20)$$

C. Discussions.

In this subsection we will compare the BOT results to the ED data. Let us first discuss the dependence of the singlet-triplet ratio $R = \frac{\Delta^S}{\Delta^T}$, where Δ^S is the singlet-singlet gap and Δ^T the singlet-triplet gap ($\Delta^T = \Delta$). It was shown in ref. [8] that, in presence of dimerization ($\delta \neq 0$) this ratio is a universal function which depends on the frustration parameter only (in the commensurate region). In fig. 4 we have plotted R for different parameter δ as a function of α . The agreement with the ED data is surprisingly good. We observe that R^{BOT} has a small dependence on δ . However, when δ is increasing $R^{BOT} \rightarrow R^{ED}$. Especially for $\alpha = 0$ we observe that $R(\alpha = 0) \rightarrow 2$. The deviation for large δ in the ED data were attributed to the crossing of the disordered line.

It was shown in ref. [8], that a well defined second triplet branch split from the continuum in the vicinity of $q = 0$ (resp. $q = \pi$) if the strength of the frustration is large enough, $\alpha > \alpha^*(\delta)$. In particular it was shown that $\alpha^*(\delta) \approx (1 - \delta)/3$. In fig.5 we have plotted α^* as a function of δ calculated exactly and within the BOT method. We find that the qualitative agreement with the ED data is very good. For large δ we have found that $\alpha_{BOT}^*(\delta) \approx 1/2\alpha_{ED}^*(\delta)$. We believe that this discrepancy on the slope is due to the fact that the width of the dispersion of the elementary triplet is underestimated in the BOT approach.

We observe that in the unfrustrated case ($\alpha = 0$) increasing δ reduces the region where the second triplet appears below the continuum. In other words, $Q_c(\delta)$, the momentum where the triplet split from the continuum, increases with δ . The variation of Q_c with δ is plotted in fig.6 and it is in agreement with eq.(20), $Q_c \rightarrow \pi/3$ when $\delta \rightarrow 1$. Thus, in the unfrustrated case, the effect of δ reduces the effective interaction between two elementary triplets excitation. In order to visualize the effect of the

frustration, we have plotted in fig.7, the dispersion of the lowest excitations, ie. the elementary triplet excitation and the two bound-states for a fixed value of the dimerization parameter. The figure shows, in agreement with the previous work [8], that the effect of the frustration increases the region where the second triplet is a well defined excitation. These figures are very similar to fig.5 of ref. [7].

V. CONCLUSIONS.

As a conclusion, using the Bond operator method we have shown that in the frustrated dimerized Heisenberg model, there is only one elementary excitation branch (lowest triplet branch). Depending on the parameters (δ, α), two bound states of these elementary excitations, one singlet and one triplet, can appear below the continuum. Even in absence of frustration the singlet bound-state is a well defined excitation for any momentum. However, in good agreement with previous work, the region where the second triplet is well defined depends on the frustration parameter. The triplet bound-state is observable in the vicinity of $q = 0$ (resp. $q = \pi$) when the frustration strength is large enough. Furthermore, in the unfrustrated case, the region where the second triplet is split from the continuum, reduces when increasing the dimerization parameter δ .

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FIG. 1. Diagrams in the ladder approximation for the vertex scattering amplitude (a), and the self-energy (b)

FIG. 2. Gap Δ as a function of α for $\delta = 0.2$ and 0.4 . The full symbols are Exact Diagonalizations data from ref. [8] (extrapolated in the thermodynamic limit). The continuous line are BOT calculations without constraint, and the dotted line with constraint.

FIG. 3. Dispersion of the lowest triplet branch for a fixed $\delta = 0.2$ and $\alpha = 0$ (a) and $\alpha = 0.3$ (b). The symbols are ED data (for a system size $L = 20$). The dashed line are BOT calculations without constraint, and the continuous line with constraint.

FIG. 4. Singlet-Triplet gaps ratio. The symbols are ED data from ref. [8]. The lines are BOT data calculated for different values of δ .

FIG. 5. α^* as a function of δ . Symbols are ED data from ref. [8], and the continuous line corresponds to BOT results.

FIG. 6. Q_c as a function of δ in the unfrustrated case.

FIG. 7. Dispersion of the triplet elementary excitation, singlet bound-state and triplet-bound-state for a fixed $\delta = 0.2$ and $\alpha = 0.1$ (a), 0.17 (b) and 0.25 (c). The continuum corresponds to the shaded region.

$$\begin{array}{c} \longrightarrow \\ \longrightarrow \end{array} \boxed{\Gamma} \begin{array}{c} \longrightarrow \\ \longrightarrow \end{array} = \begin{array}{c} \longrightarrow \\ \longrightarrow \end{array} \boxed{\mathbf{U}} \begin{array}{c} \longrightarrow \\ \longrightarrow \end{array} + \begin{array}{c} \longrightarrow \\ \longrightarrow \end{array} \boxed{\mathbf{U}} \boxed{\Gamma} \begin{array}{c} \longrightarrow \\ \longrightarrow \end{array}$$

(a)



(b)













